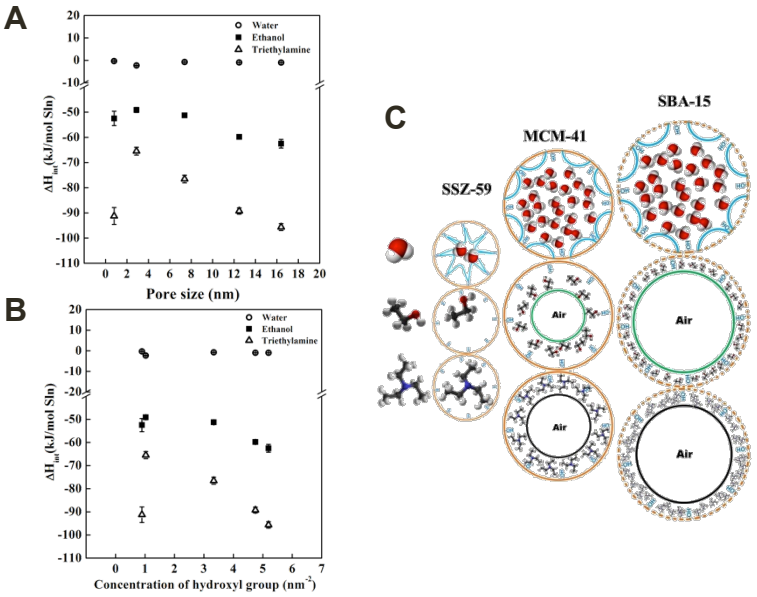
SMALL MOLECULE – SILICA INTERACTIONS IN POROUS SILICA STRUCTURES



A. Enthalpies of interaction for porous silica per mole of solution vs. pore size in water, ethanol and triethylamine.
B. Enthalpies of interaction for porous silica per mole of liquid vs. concentration of hydroxyl group per nm2 in water, ethanol and triethylamine.
C. Proposed structures of water (top), ethanol (middle) and triethylamine (bottom) in pores of SSZ-59 (left), MCM-41 (center) and SBA-15 (right). Dimensions are approximate.

Scientific Achievement

Enthalpies of immersion for calcined porous silica with different pore sizes were measured at 25 oC. Combined with TG-DSC and nitrogen adsorption analysis data, these measurements allowed interaction enthalpies of water, ethanol and triethylamine with inorganic porous silica matrices of different pore size to be calculated.

Significance and Impact

Our thermochemical results suggest that organics preferentially bond to porous silica with relatively hydrophobic surfaces. Silica with smaller pores and higher surface hydroxyl group density yield stronger guest–host interactions. The role of organic interactions at silica surfaces may be important in the CO2 sequestration environment, potentially influencing CO2 capture and carbonate precipitation.

Research Details

Immersion calorimetry, TG-DSC, nitrogen adsorption, X-ray diffraction

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